A six-stage third order additive method for stiff ordinary differential equations [*]

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Abstract

In this paper we construct a third order method for solving additively split autonomous stiff systems of ordinary differential equations. The constructed additive method is L-stable with respect to the implicit part and allows to use an arbitrary approximation of the Jacobian matrix. Automatic stepsize selection based on local error and stability control are performed. The estimations for error and stability control have been obtained without significant additional computational costs. Numerical experiments show reliability and efficiency of the implemented integration algorithm.

1 Introduction

Spatial discretization of continuum mechanics problems in partial differential equations by finite difference or finite element methods results in the Cauchy problem for the system of ordinary differential equations with an additively split right hand side function of the form:

$$y' = \varphi(t, y) + g(t, y), \quad y(t_0) = y_0, \quad t_0 \le t \le t_k,$$

where $\varphi(t, y)$ is a non-symmetrical term obtained from discretization of the first-order differential operator, $g(t, y)$ is a symmetrical term obtained from discretization of the second-order differential operator, t is a independent variable. It is assumed that in the problem the vector-function g is a stiff term and φ is a non-stiff term.

Explicit Runge-Kutta methods have a bounded stability region and are suitable for non-stiff and mildly stiff problems only. L-stable methods are usually used for solving stiff problems. In the case of large-scale problems overall computational costs of L-stable methods are almost completely dominated by evaluations and inversions of the Jacobian matrix of a right hand side vector function. Overall computational costs can be significantly reduced by re-using the same Jacobian matrix over several integration steps (freezing the Jacobian).

Freezing the Jacobian in iterative methods has effect on convergence speed of an iterative process only and doesn't lead to loss of accuracy. So, this approach is extensively used for implementation of these methods. For Rosenbrock type methods and their modifications [4] an approximation of the Jacobian matrix can lead to decreasing a consistency order.

The system $y' = f(t, y)$ can be written in the form $y' = [f(t, y) - By] + By$, where B is some approximation of the Jacobian matrix. Assume that stiffness is fully concentrated in the term $g(t, y) = By$, then the expression $\varphi(t, y) = f(t, y) - By$ can be interpreted as the non-stiff term [2, 7]. If the Cauchy problem is considered in the form $y' = [f(t, y) - By] + By$ under construction of additive methods, then an arbitrary approximation of the Jacobian matrix can be used without decreasing the

order of these methods. Additive methods constructed in this way allow both analytical and numerical computations of the Jacobian matrix. Note that the approximation of the Jacobian by a diagonal matrix is suitable for some mildly stiff problems.

In this paper we construct a six-stage third order additive method that allows to use different kinds of approximation of the Jacobian matrix. The estimations of the error and the maximum absolute eigenvalue of the Jacobian matrix have been obtained without significant additional computational costs. Indeed, the error estimation has been obtained on the base of an embedded additive method and the maximum absolute eigenvalue estimation has been obtained by a power method using only two additional computations of $\varphi(y)$. These estimations are used for error and stability control correspondingly. Numerical experiments are performed showing the reliability and efficiency of the constructed method.

2   A numerical scheme for autonomous problems

Consider the Cauchy problem for an autonomous system of ordinary differential equations

$$y' = \varphi(y) + g(y), \quad y(t_0) = y_0, \quad t_0 \leq t \leq t_k, \tag{1}$$

where y, φ and g are N-dimensional smooth vector-functions, t is an independent variable. In the following, we assume that g is a stiff term and φ is a non-stiff term. Consider a six-stage numerical scheme for solving (1):

$$
\begin{aligned}
y_{n+1} &= y_n + \sum_{i=1}^{6} p_i k_i\,, \\
k_1 &= h\varphi(y_n), \\
D_n k_2 &= h[\varphi(y_n) + g(y_n)], \\
D_n k_3 &= k_2, \\
D_n k_4 &= h\varphi(y_n + \sum_{j=1}^{3} \beta_{4j} k_j) + hg(y_n + \sum_{j=1}^{3} \alpha_{4j} k_j), \\
D_n k_5 &= k_4 + \gamma k_3, \\
k_6 &= h\varphi(y_n + \sum_{j=1}^{5} \beta_{6j} k_j),
\end{aligned}
\tag{2}
$$

where $D_n = E - ahg'_n$, $g'_n = \partial g(y_n)/\partial y$ is the Jacobian matrix of the function $g(y)$, E is the identity matrix, k_i, $1 \leq i \leq 6$, are stages, $a, p_i, \alpha_{4j}, \beta_{4j}, \beta_{6j}, \gamma$ are coefficients that have effect on accuracy and stability properties of the scheme (2).

3 The third order conditions

The Taylor series expansion of the approximate solution up to terms in h^3 has the form

$$
\begin{aligned}
y_{n+1} = {} & y_n + \big(p_1 + p_2 + p_3 + p_4 + (\gamma+1)p_5 + p_6\big)h\varphi + \big(p_2 + p_3 + p_4 + (\gamma+1)p_5\big)hg + \\
& + \Big((\beta_{41}+\beta_{42}+\beta_{43})(p_4+p_5) + \big(\beta_{61}+\beta_{62}+\beta_{63}+\beta_{64}+(\gamma+1)\beta_{65}\big)p_6\Big)h^2\varphi'\varphi + \\
& + \Big((\beta_{42}+\beta_{43})(p_4+p_5) + \big(\beta_{62}+\beta_{63}+\beta_{64}+(\gamma+1)\beta_{65}\big)p_6\Big)h^2\varphi'g + \\
& + \big[a(p_2+2p_3+p_4+(3\gamma+2)p_5) + (\alpha_{41}+\alpha_{42}+\alpha_{43})(p_4+p_5)\big]h^2 g'\varphi + \\
& + \big[a(p_2+2p_3+p_4+(3\gamma+2)p_5) + (\alpha_{42}+\alpha_{43})(p_4+p_5)\big]h^2 g'g + \\
& + 0.5\big[(\beta_{41}+\beta_{42}+\beta_{43})^2(p_4+p_5) + \big(\beta_{61}+\beta_{62}+\beta_{63}+\beta_{64}+(\gamma+1)\beta_{65}\big)^2 p_6\big]h^3\varphi''\varphi^2 + \\
& + 0.5\big[(\beta_{42}+\beta_{43})^2(p_4+p_5) + \big(\beta_{62}+\beta_{63}+\beta_{64}+(\gamma+1)\beta_{65}\big)^2 p_6\big]h^3\varphi''g^2 + \\
& + \big[(\beta_{42}+\beta_{43})(\beta_{41}+\beta_{42}+\beta_{43})(p_4+p_5) + \big(\beta_{61}+\beta_{62}+\beta_{63}+\beta_{64} + \\
& + (\gamma+1)\beta_{65}\big)\big(\beta_{62}+\beta_{63}+\beta_{64}+(\gamma+1)\beta_{65}\big)p_6\big]h^3\varphi''\varphi g + (\beta_{41}+\beta_{42} + \\
& + \beta_{43})(\beta_{64}+\beta_{65})p_6 h^3\varphi'^2\varphi + (\beta_{42}+\beta_{43})(\beta_{64}+\beta_{65})p_6 h^3\varphi'^2 g + \\
& + \Big[a\big((\beta_{42}+2\beta_{43})(p_4+p_5) + \big(\beta_{62}+2\beta_{63}+\beta_{64}+(3\gamma+2)\beta_{65}\big)p_6\big) + \\
& + (\alpha_{41}+\alpha_{42}+\alpha_{43})(\beta_{64}+\beta_{65})p_6\Big]h^3\varphi'g'\varphi + \Big[a\big((\beta_{42}+2\beta_{43})(p_4+p_5) + \\
& + \big(\beta_{62}+2\beta_{63}+\beta_{64}+(3\gamma+2)\beta_{65}\big)p_6\big) + (\alpha_{42}+\alpha_{43})(\beta_{64}+\beta_{65})p_6\Big]h^3\varphi'g'g + \\
& + 0.5(\alpha_{41}+\alpha_{42}+\alpha_{43})^2(p_4+p_5)h^3 g''\varphi^2 + 0.5(\alpha_{42}+\alpha_{43})^2(p_4+p_5)h^3 g''g^2 + \\
& + (\alpha_{42}+\alpha_{43})(\alpha_{41}+\alpha_{42}+\alpha_{43})(p_4+p_5)h^3 g''\varphi g + a(\beta_{41}+\beta_{42}+\beta_{43})(p_4 + \\
& + 2p_5)h^3 g'\varphi'\varphi + a(\beta_{42}+\beta_{43})(p_4+2p_5)h^3 g'\varphi'g + a\big[a(p_2+3p_3+p_4 + \\
& + (6\gamma+3)p_5) + (\alpha_{41}+2\alpha_{42}+3\alpha_{43})p_4 + (2\alpha_{41}+2\alpha_{42}+3\alpha_{43})p_5\big]h^3 g'^2\varphi + \\
& + a\big[a(p_2+3p_3+p_4+(6\gamma+3)p_5) + (2\alpha_{42}+3\alpha_{43})p_4 + (2\alpha_{42}+3\alpha_{43})p_5\big]h^3 g'^2 g + \\
& + O(h^4),
\end{aligned}
$$

where the corresponding elementary differentials are evaluated at y_n.
The Taylor series expansion of the exact solution up to third order terms is

$$
\begin{aligned}
y(t_{n+1}) = {} & y(t_n) + h(\varphi+g) + \frac{h^2}{2}(\varphi'\varphi + \varphi'g + g'\varphi + g'g) + \frac{h^3}{6}(\varphi''\varphi^2 + \\
& + \varphi''g^2 + 2\varphi''\varphi g + \varphi'^2\varphi + \varphi'^2 g + \varphi'g'\varphi + \varphi'g'g + g''\varphi^2 + g''g^2 + \\
& + 2g''\varphi g + g'\varphi'\varphi + g'\varphi'g + g'^2\varphi + g'^2 g) + O(h^4),
\end{aligned}
\tag{3}
$$

where the corresponding elementary differentials are evaluated at $y(t_n)$.

Comparing the successive terms in the Taylor series expansion of the approximate and the exact solutions up to third order terms under the assumption $y_n = y(t_n)$ we have the system of nonlinear algebraic equations. Its solving results in the relation $\beta_{41} = \alpha_{41} = \beta_{61} = 0$ and the third order

conditions of the scheme (2) take form:

$$\begin{aligned}
&1)\quad p_2 + p_3 + p_4 + (\gamma + 1)p_5 = 1,\\
&2)\quad (\beta_{41} + \beta_{42} + \beta_{43})(p_4 + p_5) + \big(\beta_{61} + \beta_{62} + \beta_{63} + \beta_{64} +\\
&\qquad + (\gamma + 1)\beta_{65}\big)p_6 = 0.5,\\
&3)\quad a\big(p_2 + 2p_3 + p_4 + (3\gamma + 2)p_5\big) + (\alpha_{41} + \alpha_{42} + \alpha_{43})(p_4 + p_5) = 0.5,\\
&4)\quad (\beta_{41} + \beta_{42} + \beta_{43})^2(p_4 + p_5) + \big(\beta_{61} + \beta_{62} + \beta_{63} + \beta_{64} +\\
&\qquad + (\gamma + 1)\beta_{65}\big)^2 p_6 = 1/3,\\
&5)\quad (\beta_{41} + \beta_{42} + \beta_{43})(\beta_{64} + \beta_{65})p_6 = 1/6,\\
&6)\quad a\big[(\beta_{42} + 2\beta_{43})(p_4 + p_5) + (\beta_{62} + 2\beta_{63} + \beta_{64} + (3\gamma + 2)\beta_{65})p_6\big] +\\
&\qquad + (\alpha_{41} + \alpha_{42} + \alpha_{43})(\beta_{64} + \beta_{65})p_6 = 1/6,\\
&7)\quad (\alpha_{41} + \alpha_{42} + \alpha_{43})^2(p_4 + p_5) = 1/3,\\
&8)\quad a(\beta_{41} + \beta_{42} + \beta_{43})(p_4 + 2p_5) = 1/6,\\
&9)\quad a\big[a(p_2 + 3p_3 + p_4 + (6\gamma + 3)p_5) + (\alpha_{41} + 2\alpha_{42} + 3\alpha_{43})p_4 +\\
&\qquad + (2\alpha_{41} + 3\alpha_{42} + 4\alpha_{43})p_5\big] = 1/6,\\
&10)\quad \alpha_{41} = \beta_{41} = \beta_{61} = 0,\quad p_1 = -p_6.
\end{aligned} \tag{4}$$

4   Stability analysis

The linear stability analysis of the additive scheme (2) is based on the scalar model equation

$$y' = \lambda_1 y + \lambda_2 y, \quad y(0) = y_0, \quad t \geq 0, \ \mathrm{Re}(\lambda_1) \leq 0, \ \mathrm{Re}(\lambda_2) \leq 0, \ |\mathrm{Re}(\lambda_1)| \ll |\mathrm{Re}(\lambda_2)|, \tag{5}$$

where the free parameters λ_1, λ_2 can be interpreted as some eigenvalues of the Jacobian matrices of the functions φ (the non-stiff term) and g (the stiff term) correspondingly.

Application of the scheme (2) for numerical solving the equation (5) yields

$$y_{n+1} = R(x, z)y_n,$$

where $x = \lambda_1 h$, $z = \lambda_2 h$ and $R(x, z)$ is a stability function (its analytical expression is omitted here for brevity).

The necessary condition of L-stability of the additive scheme (2) with respect to the stiff term has the form:

$$\lim_{z \to -\infty} R(x, z) = 0.$$

It is satisfied if the following two conditions hold:

$$\begin{aligned}
&a^2(p_1 + p_6) + \big((\alpha_{42} - a)\beta_{64} - a\beta_{62}\big)p_6 = 0,\\
&a(a - p_2) + (\alpha_{42} - a)p_4 = 0.
\end{aligned} \tag{6}$$

Solving the system (4), (6). In the following, we assume that $\sum_{j=1}^{3} \alpha_{4j} = 1$, $\alpha_{42} = a$, $\beta_{42} = a$. The first relation ensures that $g(y_n + \sum_{j=1}^{3} \alpha_{4j}k_j)$ approximate $g(y(t_{n+1}))$ in the fourth stage and the other ones improve stability properties of the intermediate numerical formulas.

Let us denote

$$\beta_1 := \beta_{64} + \beta_{65}, \quad \beta_2 := \beta_{63} + \beta_{64} + (\gamma + 1)\beta_{65},$$
$$\beta_3 := a\big(2\beta_{63} + \beta_{64} + (3\gamma + 2)\beta_{65}\big) + \beta_{64} + \beta_{65}, \quad \beta_4 := a + \beta_{43}.$$

Then after obvious simplifications the system (4), (6) takes the form

1) $p_2 + p_3 + \gamma p_5 = 2/3,$

2) $a\beta_4(p_4 + 2p_5) = 1/6,$

3) $\beta_4\beta_1 p_6 = 1/6,$

4) $\beta_4/3 + \beta_2 p_6 = 0.5,$

5) $\beta_4^2/3 + \beta_2^2 p_6 = 1/3,$ $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (7)$

6) $a(2\beta_4 - a)/3 + \beta_3 p_6 = 1/6,$

7) $p_4 + p_5 = 1/3,$

8) $a\big(p_2 + 2p_3 + p_4 + (3\gamma + 2)p_5\big) = 1/6,$

9) $a\Big(a\big(p_2 + 3p_3 + p_4 + (6\gamma + 3)p_5\big) + (3 - a)p_4 + (4 - a)p_5\Big) = 1/6,$

10) $\alpha_{41} = \beta_{41} = \beta_{61} = \beta_{62} = 0, \quad \alpha_{42} = \beta_{42} = a,\ \alpha_{43} = 1 - a, \quad p_2 = a,\ p_1 = -p_6.$

Let us consider the equations (1) and (7) – (10). Multiply (1) by $3a$ and subtract the result from (8). Then divide (9) by a and subtract (1) multiplied by $6a$ from it. As the result we obtain:

$$p_2 + p_3 + \gamma p_5 = 2/3,$$
$$p_4 + p_5 = 1/3,$$
$$a(-2p_2 - p_3 + p_4 + 2p_5) = 1/6 - 2a, \qquad\qquad\qquad\qquad\qquad (8)$$
$$a(-5p_2 - 3p_3 + p_4 + 3p_5) + (3 - a)p_4 + (4 - a)p_5 = (6a)^{-1} - 4a,$$
$$p_2 = a.$$

From the second equation of (8) we have $p_4 = 1/3 - p_5$. Substituting this relation and the fifth relation of (8) to the first tree equations we have

$$p_3 + \gamma p_5 = -a + 2/3,$$
$$a(-p_3 + p_5) = 2a^2 - 7a/3 + 1/6, \qquad\qquad\qquad\qquad\qquad (9)$$
$$a(-3p_3 + 2p_5) + p_5 = 5a^2 - 4a - 1 + (6a)^{-1}.$$

From the second equation of (9) we have

$$p_3 = p_5 - (12a^2 - 14a + 1)(6a)^{-1}. \qquad\qquad\qquad\qquad\qquad (10)$$

It follows from (10) and the third equation of (9) that $p_5 = (6a^3 - 18a^2 + 9a - 1)/(6a^2 - 6a)$. Substituting p_5 to (10) we obtain $p_3 = (3a^2 - 4a + 3)/(3 - 3a)$. Substituting p_5 to (10), we have $p_3 = (3a^2 - 4a + 3)/(3 - 3a)$. Then we substitute p_5 and p_3 to the first equation of (9). As the result we have $\gamma = 2a(a + 1)/(6a^3 - 18a^2 + 9a - 1)$. It follows from the second equation of (8) that $p_4 = (6a^3 - 20a^2 + 11a - 1)/(6a - 6a^2)$. From the second equation of (7) we obtain $\beta_4 = (a - 1)/(6a^3 - 16a^2 + 7a - 1)$. The fourth and fifth equations of (7) can be written in the form $\beta_2 p_6 = (3 - 2\beta_4)/6$, $\beta_2^2 p_6 = (1 - \beta_4^2)/3$. Dividing the second equation by the first one results in $\beta_2 = (2 - 2\beta_4^2)/(3 - 2\beta_4)$. It follows from here

and the fourth equation of (7) that $p_6 = (0.5 - \beta_4/3)/\beta_2$. From the third and sixth equations of (7) we obtain $\beta_1 = (6\beta_4 p_6)^{-1}$ and $\beta_3 = [1/6 - a(2\beta_4 - \beta_{42})/3]/p_6$.

Then we express the coefficients β_{63}, β_{64} and β_{65} of the scheme (2) in terms of the auxiliary parameters β_1, β_2, β_3 and β_4, that is

$$\beta_{64} + \beta_{65} = \beta_1, \quad \beta_{63} + \gamma\beta_{65} = \beta_2 - \beta_1, \quad a(\beta_{63} - \beta_{65}) = a(3\beta_2 - 2\beta_1) + \beta_1 - \beta_3. \tag{11}$$

Multiplying the second equation of (11) by a and subtracting it from the third one we obtain $\beta_{65} = [a(\beta_1 - 2\beta_2) + \beta_3 - \beta_1]/(a\gamma + a)$. It follows from here and the second equation of (11) that $\beta_{63} = \beta_2 - \beta_1 - \gamma\beta_{65}$, and from the first relation we obtain $\beta_{64} = \beta_1 - \beta_{65}$.

As the result all the coefficients of the scheme (2) are expressed in terms of one free parameter a. The coefficient a can be found from following considerations. Let $\varphi(y) \equiv 0$, that is consider the system of the form $y' = g(y)$ instead of (1). In this case the local error δ_{n+1} at point t_{n+1} can be represented in the form

$$\delta_{n+1} = h^4(c_1 g'^3 g + c_2 g'' g' g^2 + c_3 g' g'' g^2 + c_4 g''' g^3) + O(h^5),$$

where c_i, $1 \le i \le 4$, are expressed in terms of the coefficients of the scheme (2) (their expressions are omitted here for brevity).

The system $y' = g(y)$ is stiff, that is the function $g(y)$ satisfies the Lipschitz condition with a large constant. Therefore the term $c_1 h^4 g'^3 g$ makes the largest contribution to the local error. Choose $c_1 = 0$ for minimizing the local error, then we have

$$24a^4 - 96a^3 + 72a^2 - 16a + 1 = 0. \tag{12}$$

Now, the coefficients of the L-stable third order scheme (2) can be computed by the following formulas:

$$
\begin{aligned}
&\alpha_{41} = \beta_{41} = \beta_{61} = \beta_{62} = 0, && \alpha_{42} = \beta_{42} = a, \quad \alpha_{43} = 1 - a, \quad p_2 = a, \\
&\quad \gamma = 2a(a + 1)/(6a^3 - 18a^2 + 9a - 1), && p_3 = (a^2 - 4a/3 + 1)/(1 - a), \\
&p_4 = (6a^3 - 20a^2 + 11a - 1)/(6a - 6a^2), && \\
&p_5 = (6a^3 - 18a^2 + 9a - 1)/(6a^2 - 6a), && \\
&\beta_4 = (a - 1)/(6a^3 - 16a^2 + 7a - 1), && \beta_{43} = \beta_4 - a, \\
&\beta_2 = (1 - \beta_4^2)/(1.5 - \beta_4), && p_6 = (0.5 - \beta_4/3)/\beta_2, p_1 = -p_6, \\
&\beta_1 = (6\beta_4 p_6)^{-1}, && \beta_3 = [1/6 - a(2\beta_4 - \beta_{42})/3]/p_6, \\
&\beta_{65} = [a(\beta_1 - 2\beta_2) + \beta_3 - \beta_1]/(a\gamma + a), && \\
&\beta_{63} = \beta_2 - \beta_1 - \gamma\beta_{65}, && \beta_{64} = \beta_1 - \beta_{65},
\end{aligned}
\tag{13}
$$

where the coefficient a is determined from the equation (12).

This equation has the four real roots $a_1 = 0.10643879214266$, $a_2 = 0.22042841025921$, $a_3 = 0.57281606248213$ and $a_4 = 3.1003167351160$. The numerical experiments that we have done show that the root a_3 is the most suitable. Therefore computational results will be given for $a = a_3$. The

corresponding coefficients of the L -stable third order scheme (2) take the form

$$
\begin{array}{lll}
a = +0.57281606248213, & p_1 = -0.48695861160293, & p_2 = +0.57281606248213, \\
p_3 = +1.32112526220103, & p_4 = -0.09105090402502, & p_5 = +0.42438423735836, \\
p_6 = +0.48695861160293, & \alpha_{41} = 0, & \alpha_{42} = +0.57281606248213, \\
\alpha_{43} = +0.42718393751787, & \beta_{41} = 0, & \beta_{42} = +0.57281606248213, \\
\beta_{43} = -0.18882050162852, & \beta_{61} = 0, & \beta_{62} = 0, \\
\beta_{63} = +2.51499368618962, & \beta_{64} = -0.022405291307077, & \\
\beta_{65} = +0.91371881359685, & \gamma = -2.891895009239397. &
\end{array}
\tag{14}
$$

5 Local error estimation

For the error estimation we construct the embedded method of second order of the form:

$$
\begin{aligned}
y_{n+1,\,2} &= y_n + \sum_{i=1}^{4} r_i k_i + r_5 \widetilde{k_5}\,, \\
k_1 &= h\varphi(y_n), \\
D_n k_2 &= h\big(\varphi(y_n) + g(y_n)\big), \\
D_n k_3 &= k_2, \\
D_n k_4 &= h\varphi(y_n + \sum_{j=1}^{3}\beta_{4j}k_j) + hg(y_n + \sum_{j=1}^{3}\alpha_{4j}k_j), \\
D_n \widetilde{k_5} &= k_4,
\end{aligned}
\tag{15}
$$

where the coefficients r_i, $1 \le i \le 5$, should be determined, and parameters $a, \alpha_{4j}, \beta_{4j}$ are given by (13) or (14). Note that there is not a sixth stage in (15) and there is not γk_3 in the fifth stage as opposed to (2).

The Taylor series expansion of the approximate solution computed by the scheme (15) up to terms in h^2 has the form

$$
\begin{aligned}
y_{n+1,\,2} = y_n &+ (r_1 + r_2 + r_3 + r_4 + r_5)h\varphi + (r_2 + r_3 + r_4 + r_5)hg + \\
&+ \big(a(r_2 + 2r_3 + r_4 + 2r_5) + r_4 + r_5\big)h^2 g'\varphi + \big(a(r_2 + 2r_3 + r_4 + 2r_5) + \\
&+ r_4 + r_5\big)h^2 g'g + \beta_4(r_4 + r_5)h^2\varphi'\varphi + \beta_4(r_4 + r_5)h^2\varphi'g + O(h^3),
\end{aligned}
$$

where the elementary differentials are evaluated at y_n. Comparing successive terms in the Taylor series expansion of the approximate and the exact solutions up to second order terms under the assumption $y_n = y(t_n)$ we obtain the second order conditions of the scheme (15):

$$
\begin{aligned}
&1)\ \ r_1 + r_2 + r_3 + r_4 + r_5 = 1, \\
&2)\ \ r_2 + r_3 + r_4 + r_5 = 1, \\
&3)\ \ \beta_4(r_4 + r_5) = 0.5, \\
&4)\ \ a(r_2 + 2r_3 + r_4 + 2r_5) + r_4 + r_5 = 0.5,
\end{aligned}
\tag{16}
$$

where β_4 is determined by (13). Note that it follows from the first two equations of (16) that $r_1 = 0$. Now we analyze the stability of the scheme (15). Its application for numerical solving the equation (5) yields

$$
y_{n+1,\,2} = R_2(x, z)\, y_{n,\,2}\,,
$$

where $x = \lambda_1 h,\ z = \lambda_2 h$ and the stability function $R_2(x, z)$ has the form

$$R_2(x, z) = [a^3(a - r_2)z^4 - a^3(r_2 - r_4)xz^3 - a\big(4a^2 - a(3r_2 + r_3 + 2r_4) + r_4\big)z^3 +$$
$$+ a^3 r_4 x^2 z^2 + a\big(a(3r_2 + r_3 + r_4 - r_5) - r_4(\beta_4 + 1)\big)xz^2 +$$
$$+ \big(6a^2 - a(3r_2 + 2r_3 + 3r_4 + 2r_5) + r_4 + r_5\big)z^2 - a\big(a(r_4 + r_5) + r_4\beta_4\big)x^2 z +$$
$$+ \big(-a(3r_2 + 2r_3 + 3r_4 + 2r_5) + (r_4 + r_5)(\beta_4 + 1)\big)xz +$$
$$+ (-4a + r_2 + r_3 + r_4 + r_5)z + \beta_4(r_4 + r_5)x^2 + (r_2 + r_3 + r_4 + r_5)x + 1]/(1 - az)^4.$$

The necessary condition of L-stability of the additive scheme (15) with respect to the stiff term has the form:

$$\lim_{z \to -\infty} R_2(x, z) = 0.$$

It is satisfied if $r_2 = a$.

Now we consider the system (16). Dividing the third equation by β_4 and subtracting the result from second one we obtain $r_3 = 1 - a - 0.5\beta_4^{-1}$. Expressing r_4 in terms of r_5 from the third equation (16) and substituting it to the fourth equation of (16) we have $r_4 = 0.5(1 - \beta_4)(a\beta_4)^{-1} + 2 - a, r_5 = 0.5(a - 1 + \beta_4)(a\beta_4)^{-1} - 2 + a$.

As the result we have all the coefficients of the L stable embedded method (15) of second order. For the coefficients (14) we obtain

$$r_1 = 0, \qquad\qquad r_2 = +0.57281606248213, \qquad r_3 = -0.87491444843356,$$
$$r_4 = +2.82745609901376, \qquad r_5 = -1.52535771306233.$$

The embedded method (15) requires, at each integration step, only one additional backward substitution steps of Gauss elimination method and doesn't require additional computations of right hand side, evaluations and inversions of the Jacobian matrix. In the case of large-scale problems overall computational costs of the method (15) are almost completely dominated by evaluations and inversions of the Jacobian matrix. So, we obtain the error estimation based on the embedded method (15) without significant additional computational costs.

Let us denote the error estimation by

$$err_n = \max_{1 \le i \le N} \frac{|y_n^i - y_{n,\,2}^i|}{Atol_i + Rtol_i|y_n^i|},$$

where $Atol_i$ and $Rtol_i$ are the desired tolerances prescribed by the user. If $err_n \le 1$, then the computed step is accepted, else the step is rejected and computations are repeated. When $Rtol_i = 0$, the absolute error is controlled on the i-th component of the solution with the desired tolerance $Atol_i$. If $Atol_i = 0$ then the relative error is controlled on the i-th component with the tolerance $Rtol_i$.

6   Stability control and stepsize selection

In the additive method (2) for solving (1) the non-stiff term φ is treated by the tree-stage explicit Runge Kutta method (the explicit part), and the stiff term g is treated by the L-stable $(4, 2)$-method [10–12] (the implicit part). In the general case there is no guarantee that the function $\varphi(y) = f(y) - By$ is the non-stiff term in reducing $y' = f(y)$ to $y' = [f(y) - By] + By$. If some stiffness is in $\varphi(y) = f(y) - By$ (i.e. stiffness leakage phenomenon occurs) then the additional stability control of the explicit part of the scheme (2) can increase efficiency of computations for many problems. In some cases it has no a significant effect on the efficiency of the integration algorithm because of the good stability properties of the scheme (2). Therefore the choice of using or not using the additional stability control of the explicit part is given to the end-user.

We perform the stability control of the explicit part of the scheme (2) by analogy with [9]. For additive methods in opposite to explicit Runge Kutta methods it isn't possible to use previously computed stages because of peculiarity of the problem (1). Therefore instead of using the stages k_i, $1 \leq i \leq 6$, of (2) we consider the additional stages d_1, d_2 of the form:

$$d_1 = h\varphi(y_n + \alpha_{21}k_1), \quad d_2 = h\varphi(y_n + \alpha_{31}k_1 + \alpha_{32}d_1).$$

Denote $\varphi(y) = Ay + b$, where A and b are matrix and vector with constant coefficients correspondingly, then we have

$$k_1 = h(Ay_n + b), \quad d_1 = k_1 + \alpha_{21}hAk_1, \quad d_2 = k_1 + (\alpha_{31} + \alpha_{32})hAk_1 + \alpha_{21}\alpha_{32}h^2A^2k_1.$$

Assuming $\alpha_{21} = \alpha_{31} + \alpha_{32}$ we obtain

$$d_2 - d_1 = \alpha_{21}\alpha_{32}h^2A^2k_1, \quad d_1 - k_1 = \alpha_{21}hAk_1.$$

The maximum absolute eigenvalue $v_n = h|\lambda_{n\ max}|$ of the matrix hA can be approximated using the power method by the following formula:

$$v_n = |\alpha_{32}^{-1}| \max_{1 \leq i \leq N} \frac{|d_2^i - d_1^i|}{|d_1^i - k_1^i|},$$

then the stability control can be made by $v_n \leq 2$, where number 2 is an approximate length of the stability interval of the tree-stage explicit Runge Kutta method.

In the general case this estimation is quite crude because of small number of iterations of the power method and the nonlinearity of the function $\varphi(y)$. Therefore the stability control is used for limiting the stepsize growing only.

Let the approximate solution y_n is computed with the stepsize h_n. For the stepsize selection we use $err_n = O(h_n^3)$. The stepsize h_{acc} predicted by accuracy we compute by the formula: $h_{acc} = q_1 h_n$, where q_1 is a root of the equation $q_1^3 err_n = 1$. In view of $v_n = O(h_n)$, the stepsize h_{st} predicted by stability is computed by $h_{st} = q_2 h_n$, where q_2 is a root of the equation $q_2 v_n = 2$. Then the stepsize h_{n+1} predicted by accuracy and stability is selected by the formula:

$$h_{n+1} = \max[h_n, \min(h_{acc}, h_{st})].$$

The stability control of the explicit part of the scheme (2) requires, at each integration step, two additional computations of $\varphi(y)$. These computational costs are negligible for large-scale problems, but if you are sure that all stiffness is in $g(y)$ then you can take off stability control to save computational costs.

7 Numerical experiments

Further, the numerical code based on the additive method (2) (with error and stability control as well as with diagonal Jacobian approximation) is called ASODE3 (the Additive Solver of Ordinary Differential Equations).

The test problems given below have been reduced to the form $y' = (f(y) - By) + By$. All numerical computations have been performed in double precision arithmetic on IBM PC Athlon(tm) XP 2000+ with the desired tolerances of the error $Atol = Rtol = Tol = 10^{-m}$, $m = 2, 4$. The scheme (2) is of third order, therefore it is unreasonable to do numerical computations with higher tolerance.

The following four test examples are considered:

Example 1 [18].

$$
\begin{aligned}
y_1' &= -0.013y_1 - 1000y_1y_3, \\
y_2' &= -2500y_2y_3, \\
y_3' &= -0.013y_1 - 1000y_1y_3 - 2500y_2y_3,
\end{aligned} \tag{17}
$$
$$
t \in [0, 50], \quad y_1(0) = 1, \quad y_2(0) = 1, \quad y_3(0) = 0, \quad h_0 = 2.9 \cdot 10^{-4}.
$$

Example 2 [14].

$$
\begin{aligned}
y_1' &= 77.27(y_2 - y_1y_2 + y_1 - 8.375 \cdot 10^{-6}y_1^2), \\
y_2' &= (-y_2 - y_1y_2 + y_3)/77.27, \\
y_3' &= 0.161(y_1 - y_3),
\end{aligned} \tag{18}
$$
$$
t \in [0, 300], \quad y_1(0) = 4, \quad y_2(0) = 1.1, \quad y_3(0) = 4, \quad h_0 = 2 \cdot 10^{-3}.
$$

Example 3.

$$
\begin{aligned}
y_1' &= -0.04y_1 + 0.01y_2y_3, \\
y_2' &= 400y_1 - 100y_2y_3 - 3000y_2^2, \\
y_3' &= 30y_2^2, \\
t &\in [0, 40], \quad y_1(0) = 1, \quad y_2(0) = y_3(0) = 0, \quad h_0 = 10^{-5}.
\end{aligned}
$$

Example 4.

$$
\begin{aligned}
y_1' &= y_3 - 100y_1y_2, \\
y_2' &= y_3 + 2y_4 - 100y_1y_2 - 2 \cdot 10^4 y_2^2, \\
y_3' &= -y_3 + 100y_1y_2, \\
y_4' &= -y_4 + 10^4 y_2^2, \\
t &\in [0, 20], \quad y_1(0) = y_2(0) = 1, \quad y_3(0) = y_4(0) = 0, \quad h_0 = 2.5 \cdot 10^{-5}.
\end{aligned}
$$

The approximation of the Jacobian by a diagonal matrix is used when solving the test problems by ASODE3. For the first test problem the diagonal matrix B with elements $b_{11} = -0.013 - 1000y_3$, $b_{22} = -2500y_3$, $b_{33} = -1000y_1 - 2500y_2$ are used. In the case of diagonal Jacobian approximation computational costs of additive methods are dominated by the number of right hand side function evaluations. So, computational costs of (2) per integration step are comparable to ones of explicit methods. Hence, ASODE3 is compared with the following numerical codes based on well-known explicit

RKM4 – 5-stage   Merson method of order 4 [15],
RKF5 – 6-stage   Felberg method of order 5 [16],
RKF7 – 13-stage Felberg method of order 7 [16],
DP8   – 13-stage Dormand and Prince method method of order 8 [17],
and less well-known Runge-Kutta type method:
RKN2 – 2-stage   method of order 2 [13].

The overall computational costs (measured by the number of right hand side function evaluations over the integration interval) are given in the table

Table 1.
Computational costs of RKM4, RKF5, RKF7, DP8, RKN2, ASODE3 with stability control.

№	Tol	RKM4	RKF5	RKF7	DP8	RKN2	ASODE3
1	10^{-2}	401 716	401 005	982 536	717 526	222 441	243
	10^{-4}	400 627	400 656	982 150	717 287	222 481	5 253
2	10^{-2}	13 391 594	15 694 434	38 429 196	27 998 053	8 682 849	4 245
	10^{-4}	13 384 132	15 691 105	38 429 976	27 993 793	8 689 861	89 993
3	10^{-2}	204 889	237 942	587 509	431 591	133 022	1 278
	10^{-4}	206 647	240 676	565 396	430 823	132 987	7 908
4	10^{-2}	10 832	11 874	29 991	23 052	6 585	174
	10^{-4}	10 236	11 366	28 819	23 354	7 627	7 938

8   Conclusions

In addition to continuum mechanics problems, the constructed additive method can be used for solving locally unstable problems. In this case $\varphi(y)$ corresponds to eigenvalues of the Jacobian matrix with positive real parts. In opposite to A-stable methods, explicit Runge Kutta methods are unstable in almost the entire right half plane and therefore are more suitable for detecting the local unstable solutions. For many locally unstable problems it is also easy to split the right hand side into stiff and non-stiff terms from physical considerations.

So, in this paper, we constructed the third order additive method that is L-stable with respect to the implicit part and allows to use an arbitrary approximation of the Jacobian matrix without loss of accuracy. Automatic stepsize selection based on local error and stability control are performed and the auxiliary formulas for doing this were obtained without significant additional computational costs.

The aim of numerical computations was to test the reliability and efficiency of the implemented integration algorithm with error and stability control as well as with diagonal Jacobian approximation. They didn't aim at solving practical problems of continuum mechanics and locally unstable problems. Numerical experiments show reliability and efficiency of the presented method. It follows from them that the method has good stability properties for solving mildly stiff problems and that the test problems turned out to be rather stiff for the explicit Runge-Kutta methods considered above. It is worth remarking that computational costs per step are comparable for both the additive method (with diagonal Jacobian approximation) and explicit ones. So, the implemented integration algorithm makes it possible to expend the range of applicability of explicit Runge-Kutta methods towards more stiff problems.

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